

EFFECT OF POLARISATION ON THE ELASTIC ELECTRON SCATTERING BY HELIUM ATOM

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ABSTRACT. The S -wave phase-shifts (η_0) in the elastic \bar{e} -He scattering have been calculated by Hulthén's (1944) variational method taking into account polarisation effects due to the virtual excitation to 2^1S state, but neglecting exchange. The calculated phase-shift values compare favourably with those of Westin as quoted by Mott and Massey (1965).

INTRODUCTION

In problems of elastic scattering of electrons by atoms, the inclusion of the influence of exchange and polarisation effects brings in additional complications. Both the effects, due to exchange and polarisation, decrease, though differently, with increasing energy. The exchange issue arises out of the indistinguishability of the incoming and bound electrons and the polarisation effect is due to the distortion of the atomic cloud by the influence of the incoming electron.

The first theoretical attempt to investigate the \bar{e} -He elastic scattering considering exchange effect has been made by Massey and Mohr (1931). They have concluded that the inclusion of the exchange effect modifies appreciably the phase-shift below 15 ev. McDougall (1932) has computed the S -wave phase-shifts of elastic scattering of electron by helium atom neglecting exchange and polarisation effects. Using the simple Hylleraas wavefunction for the ground state of the helium atom, Morse and Allis (1933) have taken into account the exchange effect in their calculation of the same problem and have solved the resulting integro-differential equation numerically. Recently LaBahn and Callaway (1964, 1966) have carried out phase-shift computation on elastic \bar{e} -He collision taking into account both the exchange possibility and the polarisation effect. Williamson and McDowell (1965) also have solved the same problem but with an open-shell wave function. The present authors (1966) have applied the variational method to the same problem. In all these attempts, polarisation effect has been considered by properly modifying the atomic static potential part. This modification manifests itself by the presence of extra polarisation terms in addition to the already existing static potential part.

Here, however, instead of modifying the static potential to include the polarisation effect, we have taken into account the distortion of the original ground-state

wave function of the atom in the presence of the incoming electron, in analogy with our previous work (1965) on \bar{e} -H scattering to explain the resonance phenomena in the elastic electron scattering experiments of Schulz (1964). We assume that the distortion of the initial 1S state is in the form of a superposition of higher excited states induced temporarily when the incident electron is near the atom but when the electron is far away, the atom comes back to its original 1S-state. For simplicity of calculation we have considered the virtual excitation to the next higher possible state only with the same symmetry (i.e. 2'S state), as such the exchange effect has not been considered in our formulation.

THEORY

The wave-function $\bar{\Psi}(r_1, r_2, r_3)$ of the system of three electrons moving in the field of a proton satisfies the wave equation $(H-E)\bar{\Psi}(r_1, r_2, r_3) = 0$

with $H = -\frac{\nabla_1^2}{2} - \frac{\nabla_2^2}{2} - \frac{\nabla_3^2}{2} - \frac{2}{r_1} - \frac{2}{r_2} - \frac{2}{r_3} + \frac{1}{r_{12}} + \frac{1}{r_{23}} + \frac{1}{r_{13}}$ in atomic units (i.e.

$e = m = \hbar = 1 = a_0$); here r_1, r_2, r_3 are the co-ordinates of the three electrons referred to the helium nucleus, r_{12}, r_{23}, r_{13} are the distances between the two of them, E is the total energy of the system (in a.u.)

The total wave-function $\psi(r_1, r_2, r_3)$ is approximated as

$$\psi(r_1, r_2, r_3) = \chi(r_1, r_2, r_3) F(r_3) \quad (1)$$

with $\chi(r_1, r_2, r_3) = \psi_1(r_1, r_2)(1 - \alpha e^{-\lambda r_3}) + \psi_2(r_1, r_2)\beta e^{-\mu r_3}$

and χ satisfies the normalisation condition $\iint \chi^* \chi dr_1 dr_2 = 1$; hence $2\alpha = \beta^2$ and $\lambda = 2\mu$ (neglecting higher powers of β)

For convenience of calculation, we have taken $\lambda = Z$ (i.e. 27/16), the effective charge.

The trial function $F(r_3)$ is chosen in the form

$$F(r_3) = \left\{ \frac{\sin kr_3}{kr_3} + (a + be^{\mu r_3})(1 - e^{\mu r_3}) \frac{\cos kr_3}{kr_3} \right\}$$

a and b are adjustable variational parameters and k is the Wave-number of the incoming electron.

The trial wave function has the asymptotic form $\frac{\sin kr_3}{kr_3} + a \frac{\cos kr_3}{kr_3}$ and is finite at the origin. The S -wave phase-shift is given by $\eta_0 = \tan^{-1} a$.

Calculation of 'L'

The variational integral L now stands as

$$\begin{aligned} L = & -\frac{1}{2} \int \psi^*(r_1, r_2, r_3) (\nabla_1^2 + \nabla_2^2 + \nabla_3^2) \psi(r_1, r_2, r_3) dr_1 dr_2 dr_3 \\ & -2 \int \left(\frac{1}{r_1} + \frac{1}{r_2} + \frac{1}{r_3} \right) \psi^*(r_1, r_2, r_3) \psi(r_1, r_2, r_3) dr_1 dr_2 dr_3 \\ & + \int \left(\frac{1}{r_{12}} + \frac{1}{r_{13}} + \frac{1}{r_{23}} - E \right) \psi^*(r_1, r_2, r_3) \psi(r_1, r_2, r_3) dr_1 dr_2 dr_3 \end{aligned}$$

the trial wave function ψ is as given by the expression (1).

Using the eigen-value equations

$$\left(\nabla_1^2 + \nabla_2^2 + \frac{4}{r_1} + \frac{4}{r_2} - \frac{2}{r_{12}} + 2\epsilon_1 \right) \psi_1(r_1, r_2) = 0$$

$$\text{and} \quad \left(\nabla_1^2 + \nabla_2^2 + \frac{4}{r_1} + \frac{4}{r_2} - \frac{2}{r_{12}} + 2\epsilon_2 \right) \psi_2(r_1, r_2) = 0$$

where ψ_1 , ϵ_1 and ψ_2 , ϵ_2 are the wavefunctions and eigen-energies of the atom in the ground state (1S) and excited 2^1S state (singlet) respectively, we get

$$\begin{aligned} -2L = & \int \left(1 - \frac{\beta^2}{2} e^{-\mu r_3} \right) F(r_3) \left(\nabla_3^2 + \frac{4}{r_3} + 2E - 2\epsilon_1 \right) \left(1 - \frac{\beta^2}{2} e^{-\mu r_3} \right) F(r_3) dr_3 \\ & + \beta^2 \int e^{-\mu r_3} F(r_3) \left(\nabla_3^2 + \frac{4}{r_3} + 2E - 2\epsilon_2 \right) e^{-\mu r_3} F(r_3) dr_3 \\ & + 4\beta^2 \int (\psi_1^2 - \psi_2^2) \left(\frac{1}{r_{13}} e^{-2\mu r_3} F^2(r_3) dr_1 dr_2 dr_3 \right. \\ & \left. - 8\beta \int \psi_1 \psi_2 \frac{1}{r_{13}} e^{-\mu r_3} F^2(r_3) dr_1 dr_2 dr_3 \right. \\ & \left. - 4 \int \psi_1^2 \frac{1}{r_{13}} F^2(r_3) dr_1 dr_2 dr_3 \right) \end{aligned}$$

To evaluate the above explicitly, properly orthogonal analytic (approximate).

functions for the ground state and excited state have been used (Marriott, 1957). They are as follows :

$$\psi_1(r_1, r_2) = \frac{z^3}{\pi} e^{-Z(r_1+r_2)}$$

$$\psi_2(r_1, r_2) = C[e^{-2r_1}(e^{-fr_2} - gr_2e^{-hr_2}) + e^{-2r_2}(e^{-fr_1} - gr_1e^{-hr_1})]$$

where $C = \frac{2^{1/4} \times .478}{\pi}$; $f = 1.136$, $g = .317$ and $h = .464$.

The variational method due to Hulthén starts from the integral $L = \int \psi^*(H-E)\psi dr_1 dr_2$. The value of the phase-parameter a is obtained from the following set of equations

$$L(\beta; b, a) = 0$$

$$\frac{\partial L}{\partial \beta} = 0$$

$$\frac{\partial L}{\partial b} = 0$$

It is to be noted that cubes and higher powers of β in L have been neglected.

The evaluation of L is now straight forward, though extremely tedious, the numerous integrals occurring therein can finally be reduced to the following three types :

$$A_{\nu\lambda} = \int_0^\infty (r)^\nu e^{-\lambda r} dr$$

$$B_{\nu\lambda} = \int_0^\infty (r)^\nu e^{-\lambda r} \cos 2kr dr$$

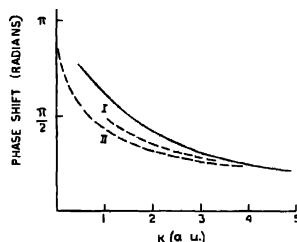
$$C_{\nu\lambda} = \int_0^\infty (r)^\nu e^{-\lambda r} \sin 2kr dr$$

In the low energy region we first find the solutions of the quadratic equation $L = 0$ obtained by putting $\beta = 0$. One of the solutions agrees with the results of McDougall (1932). Now to find the required solution of the fourth degree equation at low energy we search for the root in the neighbourhood of the particular solution mentioned above; a root is obtained differing only slightly from the particular solution chosen of the quadratic equation. Once the root has been fixed for a particular low energy, the phase-shifts for higher energies have been obtained by solving the fourth degree equation and using the continuity property of the phase-shift.

RESULTS AND DISCUSSIONS

We have evaluated the S -wave phase-shift values for the case $b = 0$ in the trial function $F(r_3)$ for energies ranging from 13.6 eV to 160.6 eV by using only the coupling of $1S$ and the virtually excited 2^1S state.

We have given a plot of η_0 against K in the figure. We find that present values of η_0 agree favourably with the experimental values. Recently Schulz (1966) and Kuyatt *et al.* (1965) have observed resonances in the elastic electron scattering by helium at energy 19.3 ± 1 eV. Due to the close coupling of 2^1S and 2^3S states, it is quite likely that resonance effect cannot be reproduced in this formalism, where we have neglected the contribution due to the exchange effect thus excluding the possibility of virtual excitation to the 2^3S state (cf Mott and Massey, 1965).



The S -wave phase-shift η_0 for elastic scattering of electron by helium atom plotted against K .

— derived from observed data by Westin as quoted by Mott and Massey (1965);

I—Present Calculation.

II—Calculation from the Hartree field without allowance for exchange as quoted by Mott and Massey (1965).

It may be of interest to compare the present values of η_0 with those of LaBahn and Callaway (1964), who took into account the polarisation effect by modifying the static atomic potential. At the energy 54.4 eV, η_0 calculated by the present authors is 1.16 radians, whereas the corresponding value of LaBahn and Callaway (1964) is 1.36 radians whereas the experimental value is about 1.24 radians.

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